Multi-scale modeling of an annular structured catalytic reactor: application to steam methane reforming

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Structured catalytic reactors have shown potential to intensify catalytic processes. An optimized flow pattern allows increased heat transfer and reduced pressure drop compared to conventional packed bed reactors [1-2]. A thin layer of catalyst is coated on the internals of the reactor, allowing high catalyst effectiveness factors. Reactor design, optimization and scale-up requires the development of a detailed reactor model accounting for intrinsic reaction kinetics and transport phenomena. A multi-scale approach is presented for the case of an annular structured reactor for methane steam reforming (ZoneFlow™ Reactor Technologies).

The intrinsic kinetics of steam methane reforming and water-gas shift reactions on a new Ni-based, intrinsically bound thin-layered catalyst adhered on a metal substrate were experimentally studied [3]. The experiments were performed in a tubular packed bed micro-reactor, designed to avoid transport phenomena limitations [4]. Estimation of the parameters and discrimination between the competing models followed from non-linear regression and statistical and physicochemical testing [5-7]. Intra-catalyst diffusion limitations were accounted for using a pseudo-continuum model [8].

The commercial reactor performance is also determined by the complex flow pattern. A Computational Fluid Dynamics (CFD) model was developed. The Reynolds-Averaged Navier-Stokes (RANS) approach was adopted and turbulence was accounted for through the k-ε model. Thermal conduction in the walls and the internals of the reactor was accounted for and radiation was described by means of the Rosseland-Weighted Sum of Gray Gases Model. The CFD code was coupled with the intrinsic kinetic model and effectiveness factors independently calculated were imposed. The model parameters were determined from a combination of cold flow pressure drop tests and hot inert and reactive flow tests in different pilot plant units. The complete model was finally used to perform simulations of a commercial steam reformer. Comparison with a conventional packed bed reactor is made [8-10] to demonstrate the process intensification potential of the annular structured reactor.

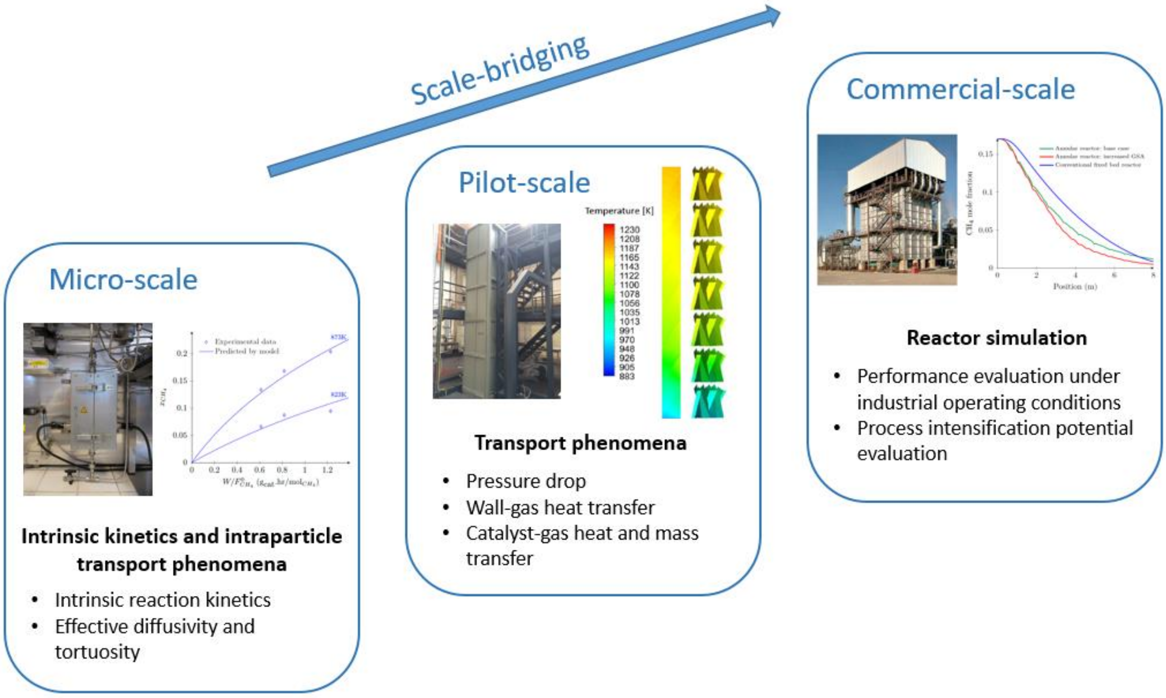

Figure 1: Multi-scale approach for the development of a reactor model.

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